0354

REPORT DOCUMENTATION PAGE
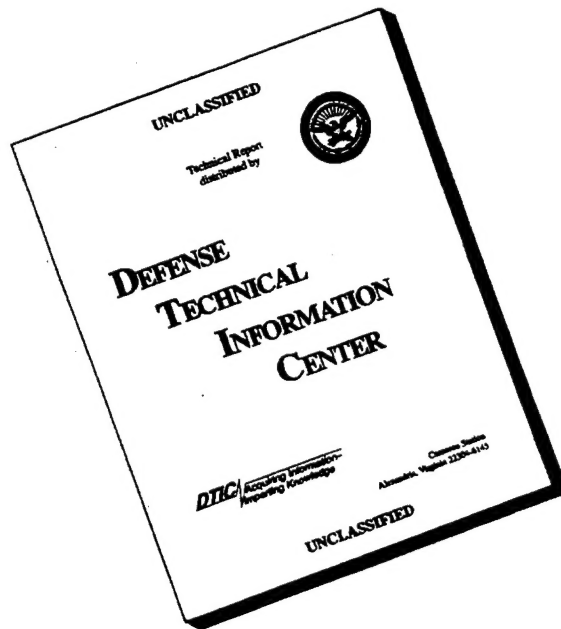
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE 4/30/96	3. REPORT TYPE AND DATES COVERED Final Report 7/1/93-4/30/96

4. TITLE AND SUBTITLE Numerical Modelling of Crystal Growth	5. FUNDING NUMBERS F49620-93-1-0521

6. AUTHOR(S)

John Strain

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Center For Pure and Applied Mathematics University of California Berkeley, CA 94720	8. PERFORMING ORGANIZATION REPORT NUMBER 1-443964-22532

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research 110 Duncan Avenue Suite B115 Bolling Air Force Base Washington, D.C. 20332-0001	10. SPONSORING/MONITORING AGENCY REPORT NUMBER F49620-93-1-0521

nm

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.	12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

19960726 030

14. SUBJECT TERMS			15. NUMBER OF PAGES 7 pages
			16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT unclassified	20. LIMITATION OF ABSTRACT none

NSN 7540-01-280-5500

DTIC QUALITY INSPECTED 1

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102

DISCLAIMER NOTICE

UNCLASSIFIED

Technical Report
distributed by

**DEFENSE
TECHNICAL
INFORMATION
CENTER**

DTIC Acquiring Information-
Imparting Knowledge

Cameron Station
Alexandria, Virginia 22304-6145

UNCLASSIFIED

THIS DOCUMENT IS BEST
QUALITY AVAILABLE. THE
COPY FURNISHED TO DTIC
CONTAINED A SIGNIFICANT
NUMBER OF PAGES WHICH DO
NOT REPRODUCE LEGIBLY.

Final Report 1993-6
AASERT Grant No. FDF49620-93-1-0053

0521

John Strain
Department of Mathematics
University of California, Berkeley

April 2, 1996

This grant supported research by two UC Berkeley graduate students on computational fluid dynamics and materials science. Both are developing innovative numerical methods for flows around complex boundaries such as occur in solidification from the melt. Research summaries for each student follow.

Ricardo Cortez (currently an NSF postdoctoral fellow at Courant Institute) studied magnetization methods for fluid flow.

A new formulation of 3-dimensional incompressible fluid flow has been presented recently with the introduction of a new variable sometimes referred to as "velocity magnetization" or simply "magnetization." A discretization of the resulting equations produces a Hamiltonian system which, in turn, leads to a new family of Lagrangian numerical methods for the study of incompressible flow. These numerical methods are essentially independent of spatial dimension and have the property that they preserve discrete invariants associated with the Hamiltonian. However there are many issues related to this new formulation that require further investigation in order to arrive at efficient numerical algorithms that may be used in a variety of situations. These issues include:

1. *The design of robust hybrid methods using vorticity and magnetization variables.* The magnetization variables can be used in conjunction with vortex methods in order to exploit the advantages that each representation offers. Accurate and relatively inexpensive procedures to switch from one computational variable to the other are required.

2. *Procedures to ensure that the magnetization remains optimal or nearly optimal.* For a given initial configuration, magnetization naturally tends to evolve into allowable configurations that depart from the optimal one. In three dimensions, finding the latter is a problem related to finding minimal surfaces attached to a fixed frame. The accuracy of the numerical method is related to the distribution of magnetization, making the problem of finding the optimal configuration a crucial part of the method.

1

3. *Applicability of these methods near boundaries.* The formulation of the Navier-Stokes equations in terms of magnetization has the potential of suggesting new ways of dealing with creation of vorticity inside boundary layers.

4. *Desingularization of the equations of motion and appropriate fast summation techniques.* The differential equations that govern the evolution of the particle positions and the magnetization they carry have high-order singularities, $O(r^{n+1})$ where n is the dimension of the problem. The order of the singularities has an adverse effect on the speed up attained by some fast summation techniques; therefore, an effort must be made to reduce the order of the singularities in the equations and to develop fast summation procedures that are well suited for these equations.

5. *Mathematical theory.* The relationship between parameters of the method and other necessary conditions for the convergence of the discrete variables to their continuous counterparts are only conjectured. There is a need for theory that provides convergence and stability proofs and error bounds based on discretization parameters.

During the academic years 1993-94 and 1994-95, this AASERT grant supported intensive work on some of the above issues, continuing the work on vortex methods which was done under the support of AFOSR Grant No. FDF49620-93-1-0053 during the last few years. A summary of Dr. Cortez's results follows.

In two dimensions, the relationship between discrete magnetization variables and vortices has been established by a rigorous interpretation of magnetization as vortex dipoles with a prescribed dipole moment. For a given discretization, each magnetization vector can be replaced by a pair of vortices of equal but opposite strength located some small distance apart. Then, vortices sufficiently "near" others can be combined into a single vortex with strength equal to the sum of individual strengths. This collapse of vortices keeps the computation feasible. Error analysis provides a criterion for how near vortices should be in order to be combined. The distance between the vortices is a parameter which is chosen so that the error in this procedure is of a prescribed size.
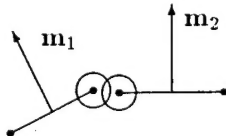
Example of combination of vortices

The reverse procedure has also been accomplished. Given a set of vortices of net vorticity zero, one can extract subsets to be represented by a string of vortex pairs, which are then approximated by magnetization vectors. The errors in both procedures are shown to be $O(h^2)$, where h is the dipole distance.

The ability to switch from magnetization to vorticity and back allows numerical experiments that compare particle positions obtained by magnetization methods with those obtained by well understood vortex methods, and provides a very important first step toward the making of hybrid methods. The numerical experiments show the order of convergence.

In many physical situations, a magnetization configuration, which initially represents a given set of vortices to a prescribed accuracy, evolves naturally in a way that endures accuracy loss to the point where the magnetization no longer approximates the original vortices evolved in time. The velocity field due to a string of magnetization vectors connecting two vortices has been interpreted as an approximation to the line integral that represents the velocity field due to the vortices. The loss of accuracy is now understood as the deterioration of the approximate line integral due to the stretching of the curve along which we integrate. This understanding has led to various procedures that correct the problem and ensure that the magnetization remains optimal by maintaining the initial accuracy over time. Some of these procedures periodically discard the integration curve and replace it with a more convenient one, computing a new magnetization field along the new curve. Others use the original curve but refine the intervals used in the quadrature so as to maintain the initial accuracy. The latter case is less efficient since the number of particles may grow without bound, but it has a natural extension to 3-dimensional problems. There, a magnetization vector is approximated by a vortex loop on the plane normal to the vector; these loops can be split into smaller ones to maintain the accuracy of the discretization. The first draft of the work above has been written as part of Mr. Cortez's dissertation.

Magnetization variables are particularly well suited for problems in which vortex dipoles are used. One such problem is the motion of an elastic membrane immersed in a fluid, where the effects of elastic forces acting on the fluid can be introduced as the rate of change of magnetization. The forces that the membrane imparts on the fluid over a small time interval represent impulse, and their effect can be introduced via vortex dipoles. In other words, the forces represent an evolving magnetization field on the membrane. This application has been implemented in two dimensions for smooth membranes and inviscid, incompressible flow.

$I\!\!R^2$ is thought of as a starting point for the understanding of magnetization and for providing extensions to $I\!\!R^3$. In three dimensions, magnetization variables have the advantage over vortex methods of automatically yielding a divergence-free vorticity field. This is a source of problems with 3-D vortex methods. Problems with 3-D magnetization methods include the arbitrary shape of the loops when two neighboring loops must be combined, and the need to find minimal surfaces when a new magnetization representation of large vortex loops is needed. Computationally efficient extensions of the 2-dimensional results will provide a promising arena for the modeling of 3-dimensional fluid flow.

3

Hans Johansen is a doctoral candidate in the Department of Mechanical Engineering at the University of California, Berkeley. His research focuses on finite difference methods for simulation of unsteady fluid dynamics, especially in bulk Czochralski crystal growth of multi-component semiconductor substrates. One of the major factors that limits the quality of such crystals, is the effect of convection in the melt on thermal gradients and composition in the solid phase (for example, see Derby [2]). By accurately representing the melt interface, fluid dynamics, and heat transfer, one can better predict crystal characteristics based on the furnace geometry and thermal environment. In addition, because the growth process is lengthy, there is the possibility of active control of certain crucible factors, such as applied magnetic fields and time-dependent heating.

Mr. Johansen's approach is based on previous work with "Cartesian grid" and "volume-of-fluid" methods for unsteady fluid dynamics. These methods represent the problem on a square finite difference grid and apply standard discretization techniques to the interior of the domain. Near irregular boundaries, on a smaller number of points, special algorithms are used to advance the solution, taking the local geometry into account. These Cartesian grid methods were recently applied to inviscid compressible flows by Pember, et al.[3]. Time step constraints (due to small cells) were overcome by redistributing excess fluxes to larger neighboring cells, while also maintaining conservation. The approach also includes AMR, local Adaptive Mesh Refinement of the finite-difference grid, based on work done by Berger and Colella [4]; results for two- and three-dimensional regions compare well with other, more expensive computations. A similar approach has been developed for incompressible flows by Almgren et al. [13], which included efficient solution of a Poisson equation, with no-flux boundary conditions, on the irregular domain. Volume-of-fluid algorithms have been applied to a number of problems in compressible flow. Chern and Colella [5] implemented conservative interface tracking for compressible flow, using a Simple Line Interface Calculation (SLIC), to represent the boundary between different gases. When combined with AMR, the method produced excellent correlation with experiments of shocks impinging on gas interfaces [6], even with the first-order representation of the front. Since then, similar volume-of-fluid algorithms have been developed for multifluid compressible flows [7], even including combustion [8], and complicated physical domains [9].

These papers demonstrate that modeling the melt motion is certainly within the capabilities of a volume-of-fluid method. The largest hurdle in applying it to crystal growth is developing an algorithm for tracking the interface, while maintaining conservation of energy. Once this is accomplished, a multi-step, predictor-corrector algorithm can be used to advance the solution in time, in which both the melt interface and container geometry will be represented using a hybrid front-tracking method derived from work mentioned above. Combining the Stefan problem with an integrator for the Boussinesq equations for the melt (similar to recent progress for incompressible flows [11, 13, 14]), will be the last step for the base algorithm. Adding an adaptive, finite-difference grid

4

hierarchy will provide local refinement of interfaces, and help verify the method. Implementation of the complex algorithm is simplified with the use of hybrid C++ and *Fortran* libraries developed at Lawrence Livermore National Labs.

The details of the method are based on the papers mentioned above, with adaptations and improvements for the Stefan problem. Our front reconstruction algorithm will be based on work done by Pilliod and Puckett [10]. Their approach provides a method of approximating an interface, based on a linear, least-squares fit to the local array of volume fractions. The algorithm is shown to be second-order accurate in space, even when applied to complicated shapes. For the Stefan problem, the interface moves normal to itself, with a speed proportional to the local temperature gradient. Chern and Colella [5] implemented shock tracking for compressible flow, which is directly applicable to the motion of the front in the Stefan problem. By coupling the reconstruction algorithm with an operator-split version of this front-tracking scheme (modified to be minimum and maximum preserving), we will be able to advance the phase boundary in time. Conservation of energy is enforced by adding equivalent heat sources, due to enthalpy of formation, where necessary.

Solving the temperature equation on the irregular, changing domain will be the next step. First, the half-time velocities will be found using an algorithm similar to those in [13]. An intermediate MAC projection guarantees that the edge-centered velocities have zero discrete divergence, making them ideal for computing a time-centered, temperature convection term. This will then be used in the right-hand side of the temperature equation, along with the enthalpy of formation mentioned earlier. The melting point of the substance will require a Dirichlet boundary condition for temperature on the interface; however, prescribing the front motion is equivalent to specifying the temperature gradient at the interface, too. This conflict will be surmounted by ignoring the constraint on the temperature gradient; it is determined by fitting a quadratic through values interpolated from full cells near the interface, using the normal and midpoint of the reconstructed front. The implicit discretization of the diffusion equation will be solved using multi-grid iterations to accelerate convergence [11] [12] . Once the new temperature field is determined, the energy loss due to a mismatch in gradients will be added into the temperature equation on the next time step.

Finally, the front position and temperature fields will be used in the integration of the Boussinesq equations for flow in the melt. The remainder of the algorithm is similar to that presented in [13] and [14]. The main differences will be the inclusion of viscosity, which demands no-slip boundary conditions at all interfaces. The viscous forces will be treated similarly to the heat equation, with the advection terms and body forces (due to gravity and externally applied magnetic fields) serving as sources in the Crank-Nicholson-type discretization. In the final step, the velocity field will be projected onto its divergence-free part.

Progress to date has focussed on accurate integration of the Stefan problem, and the heat equation with Dirichlet-type boundary conditions. First,

5

Mr. Johansen has thoroughly tested a one-dimensional method for the classical Stefan problem, which represents a balance between heat conduction and enthalpy of formation. The interface gradient is calculated using a quadratic fit to nearby temperature values; after the front is advanced, conservation is enforced by adding appropriate source terms. The quadratic temperature fit and lagged conservation have been shown to be stable for certain discretizations; results demonstrate second-order convergence in space, and first-order accuracy in time, regardless of Stefan number. Second, the solution of Dirichlet-type Poisson problems on irregular, two-dimensional domains, provides part of the time-stepping algorithm for the Stefan problem in more than one dimension. The calculation of interface gradients, based on quadratic fits to interior values, has been demonstrated as globally second-order accurate, even for front representations containing arbitrarily small cells.

Mr. Johansen will have a working code by December, 1996. Adaptive solution of the Stefan problem in multiple dimensions will be finished by June, 1996; it will provide the crucial step needed to incorporate the front motion into a Cartesian grid, incompressible Navier-Stokes solver, which is being developed at both UC Berkeley and LLNL, and will be completed by September, 1996. The remaining three months will be spent testing the algorithm, by verifying it against experimental and computational results; externally-applied magnetic fields might be included in the model in Spring of 1997. This work will be a major step in applying finite-difference algorithms to real engineering problems. The simulation of semiconductor substrate crystal growth will be a new application of the Cartesian grid method, with front tracking, convection of heat and melt composition, and adaptive refinement of the finite-difference grid around significant features.

References

[1] R. Cortez, "An Approximation to Fluid Motion Due to Boundary Forces Using Impulse Variables," *J. Computational Physics*, vol. 122, 1996, pp. 178-204.

[2] J. Derby, "An Overview of Convection During the Growth of Single Crystals from the Melt," Army High Performance Computing Research Center Preprint 92-074, 1992.

[3] R. B. Pember, J. B. Bell, P. Colella, W. Crutchfield, and M. L. Welcome, "An Adaptive Cartesian Grid Method for Unsteady Compressible Flow in Irregular Regions," *J. Computational Physics*, vol. 120, 1995, pp. 278-304.

[4] M. J. Berger and P. Colella, "Local Adaptive Mesh Refinement for Shock Hydrodynamics," *J. Computational Physics*, vol. 82, 1989, pp. 64-84.

[5] L. Chern and P. Colella, "A conservative front tracking method for hyperbolic conservation laws," Lawrence Livermore National Labs Technical Report UCRL-97200, 1987.

[6] L. F. Henderson, P. Colella, and E. G. Puckett, "On the refraction of shock waves at a slow-fast gas interface," *J. Fluid Mechanics,* vol. 224, 1991, pp. 1-27.

[7] P. Colella, H. M. Glaz, and R. E. Ferguson, "Multifluid Algorithms for Eulerian Finite Difference Methods," to appear.

[8] J. B. Bell, P. Colella, J. S. Greenough, and D. L. Marcus, "An Multi-Fluid Algorithm for Compressible, Reacting Flow," in Proceedings, AIAA 12th Computational Fluid Dynamics Conference, San Diego, CA, June 19-22, 1995.

[9] J. S. Greenough, V. Beckner, R. B. Pember, W. Y. Crutchfield, J. B. Bell, and P. Colella, "An Adaptive, Multi-Fluid, Interface-Capturing Method for Compressible Flow in Complex Geometries," in Proceedings, AIAA 26th Fluid Dynamics Conference, San Diego, CA, June 19-22, 1995.

[10] J. E. Pilliod, Jr. and E. G. Puckett, "Second-Order Volume-of-Fluid Algorithms for Tracking Material Interfaces," preprint, 1993.

[11] J. Bell, P. Colella, and M. Lai, "An Approximate Projection Method for the Incompressible Navier-Stokes Equations," to appear.

[12] W. Briggs, "A Multigrid Tutorial," SIAM, Philadelphia, PA, 1987.

[13] A. Almgren, J. B. Bell, P. Colella, and T. Marthaler, "A Cartesian Grid Projection Method for the Incompressible Euler Equation in Complex Geometries," Lawrence Livermore National Labs Technical Report UCRL JC-118091, 1994.

[14] A. Almgren, J. B. Bell, P. Colella, and L. Howell, "An Adaptive Projection Method for the Incompressible Euler Equations," Lawrence Livermore National Labs Technical Report UCRL JC-113853, 1993.